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# Monte Carlo difference schemes for the wave equation

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**Abstract** — The paper is concerned with Monte Carlo algorithms for iteration processes. A recurrent procedure is introduced, where information on various iteration levels is stored. Stability in the sense of boundedness of the correlation matrix of the component estimators is studied. The theory is applied to difference schemes for the wave equation. The results are illustrated by numerical examples.

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## 1. Introduction

An important field of application of Monte Carlo algorithms is the numerical treatment of partial differential equations. These algorithms are based on probabilistic representations expressing solutions in form of functionals on trajectories of appropriate stochastic processes (cf., e.g., [10], [12]).

If the partial differential equation is replaced by some discrete approximation in time and space, then the stochastic process reduces to a Markov chain on the corresponding grid. This relationship between difference schemes and random walks was first studied in the classical paper [5]. In the case of the heat flow equation the Markov chain is very simple. At each step the random walker goes down to the next lower time level jumping with equal probability to one of the neighbouring grid points in the space. If the walker reaches the boundary or the lowest time level, then the corresponding initial and boundary conditions are taken into account.

Stochastic algorithms of this type are well understood for partial differential equations of elliptic and parabolic type (cf., e.g., [1], [8, Ch.7, §3], [23], [11, Ch.5]). Monte Carlo and quasi-Monte Carlo methods are also successfully applied to several classes of nonlinear equations (see [18], [19], [27], [2], [4]). In case of second order hyperbolic equations, as the wave equation, the situation is quite different. Except some special situations, there are

no probabilistic representations, and the construction of efficient stochastic algorithms is a challenging task. **The purpose of the paper** is to make some steps into this direction, extending the range of applicability of the Monte Carlo method. The paper is organized as follows.

**Section 2** is concerned with Monte Carlo algorithms for iteration processes providing a general framework for difference schemes. Random walk interpretations of iteration methods have been considered, e.g., in [14]. In the classical theory of difference scheme the problem of stability of numerical algorithms is an important issue. If the dimension of the problem is sufficiently high, then Monte Carlo estimators become an efficient tool (cf. [6]). In this case the algorithm has to be stable not only with respect to round-off errors but also with respect to random errors occuring in the simulation process. We introduce the notion of stability of a Monte Carlo procedure as boundedness of the correlation matrix of the component estimators. A related notion was used in [9]. Then we first describe the classical von Neumann-Ulam scheme for solving systems of linear algebraic equations. Second we consider the direct Monte Carlo algorithm, where just one random walker is involved, and find stability conditions. Finally, we introduce a recurrent Monte Carlo algorithm, where in general many random walkers are used, and information on various iteration levels is stored. Here we prove our **main result** providing a necessary and sufficient condition for stability of the recurrent procedure.

In **Section 3** we apply the general theory to difference schemes. First we consider our main example, the wave equation. Concerning difference schemes for the wave equation we refer to [16], [7]. The recurrent procedure for the standard implicit scheme turns out to be stable, while the direct procedure is unstable. For comparison we consider the heat flow equation as a second example. Here both procedures fulfil the stability condition. Finally, we discuss numerical aspects of the theoretical results. Numerical tests for the implicit difference scheme for the one-dimensional wave equation are presented. They illustrate the phenomena of stability and instability of the recurrent procedure. It is shown that the theoretical results are useful for the prediction of the qualitative behaviour of the algorithm.

Conclusions are given in **Section 4**. In particular, the important issue of parallelization of the Monte Carlo algorithms is discussed. The proofs of some technical lemmas are collected in an **Appendix**.

## 2. Monte Carlo algorithms for iteration processes

Consider **iteration processes** of the form

$$x^n = A_0 x^n + A_1 x^{n-1} + A_2 x^{n-2} + f\,, \qquad n \geq 2\,, \tag{2.1}$$

where $x^0, x^1 \in \mathcal{R}^m$ are given initial values. A major field of application of such processes are **difference schemes** for partial differential equations. In this case the dimension $m$ of the matrices $A_0, A_1, A_2$ and of the vectors $f, x^n$ depends on the grid size in the space, while the iteration index $n$ is related to the discrete time step. The iteration process may stop at a finite number $\bar{n}$ depending on the length of the corresponding time interval and the time step. An iteration process of the form (2.1) also appears in connection with the solution of a **linear algebraic system** $x = Ax + f$, if one defines an approximation procedure using a representation $A = A_0 + A_1 + A_2$.

Two-step iteration processes of the form (2.1) can be transformed into a one-step process by considering the equivalent system (cf. [25, p. 363])

$$\begin{pmatrix} x^n \\ x^{n-1} \end{pmatrix} = \begin{pmatrix} A_0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x^n \\ x^{n-1} \end{pmatrix} + \begin{pmatrix} A_1 & A_2 \\ I & 0 \end{pmatrix} \begin{pmatrix} x^{n-1} \\ x^{n-2} \end{pmatrix} + \begin{pmatrix} f \\ f \end{pmatrix}$$

or

$$y^n = \mathcal{A}_0 y^n + \mathcal{A}_1 y^{n-1} + \varphi ,$$

where

$$y^n = \begin{pmatrix} x^n \\ x^{n-1} \end{pmatrix}, \quad \mathcal{A}_0 = \begin{pmatrix} A_0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{A}_1 = \begin{pmatrix} A_1 & A_2 \\ I & 0 \end{pmatrix}, \quad \varphi = \begin{pmatrix} f \\ f \end{pmatrix}. \tag{2.2}$$

One obtains

$$y^n = (\mathcal{I} - \mathcal{A}_0)^{-1} \mathcal{A}_1 y^{n-1} + (\mathcal{I} - \mathcal{A}_0)^{-1} \varphi \tag{2.3}$$

and

$$(\mathcal{I} - \mathcal{A}_0)^{-1} \mathcal{A}_1 = \begin{pmatrix} (I - A_0)^{-1} & 0 \\ 0 & I \end{pmatrix} \mathcal{A}_1 = \begin{pmatrix} (I - A_0)^{-1} A_1 & (I - A_0)^{-1} A_2 \\ I & 0 \end{pmatrix}. \tag{2.4}$$

The study of appropriate Monte Carlo algorithms for performing calculations according to (2.1) is of considerable interest, when the dimension $m$ is sufficiently high. Such algorithms consist of a sequence of random **estimators** $\eta^n$ for the calculation of $x^n$. In this situation an important issue is the control of the stochastic error for large $n$. Therefore, we are interested in such procedures, where the covariance matrices $\mathrm{Cov}(\eta^n)$ remain bounded as $n \to \infty$, i.e.

$$\sup_n \|\mathrm{Cov}(\eta^n)\| < \infty . \tag{2.5}$$

This property is called **stability** of the Monte Carlo algorithm.

In the first part of this section we consider the well-known von Neumann-Ulam scheme, which provides a class of estimators for inverting matrices. In the second part we study stability properties of a Monte Carlo algorithm, where the von Neumann-Ulam scheme is applied directly to the linear algebraic equation related to (2.1). In the third part we introduce a recurrent Monte Carlo algorithm, which occurs when the von Neumann-Ulam scheme is applied on each iteration step, and the obtained information is stored. We find a necessary and sufficient condition for the stability of this procedure.

## 2.1. The von Neumann-Ulam scheme

This scheme provides Monte Carlo estimators for linear functionals $(h, x)$ of the solution to equation

$$x = Ax + f , \tag{2.6}$$

where $x, f, h \in \mathcal{R}^m$, $A$ is an $m \times m$–matrix, and $(.,.)$ denotes the scalar product. Assuming convergence of the successive approximations the solution is represented as

$$x = (I - A)^{-1} f = \sum_{k=0}^{\infty} A^k f . \tag{2.7}$$

Estimators $\zeta(h, A, f)(\omega)$ are defined on the trajectories

$$\omega = (i_0, i_1, \ldots, i_k), \quad k = 0, 1, \ldots, \tag{2.8}$$

of a Markov chain with the state space $\{1, 2, \ldots, m\}$. The chain is determined by the **initial distribution** $\pi$ with

$$\sum_{i=1}^{m} \pi_i = 1, \qquad \pi_i \geq 0, \quad i = 1, \ldots, m,$$

and the **transition matrix** $P$ with

$$\sum_{j=1}^{m} p_{i,j} \leq 1, \qquad p_{i,j} \geq 0, \quad i, j = 1, \ldots, m,$$

where

$$g_i = 1 - \sum_{j=1}^{m} p_{i,j}, \qquad i = 1, \ldots, m,$$

is called the **probability of absorption**. The parameters $\pi$ and $P$ of the Markov chain are assumed to be such that the length $k = k(\omega)$ of the trajectories is finite with probability one. Moreover, they are adjusted to the parameters of the equation (2.6) by the assumptions

$$\pi_i > 0 \quad \text{if} \quad h_i \neq 0, \tag{2.9}$$

$$p_{i,j} > 0 \quad \text{if} \quad a_{i,j} \neq 0, \tag{2.10}$$

and

$$g_i > 0 \quad \text{if} \quad f_i \neq 0. \tag{2.11}$$

**Remark 2.1** *We use the notations* $|f|$, $\frac{f^2}{g}$, $|A|$, $\frac{A^2}{P}$ *for vectors and matrices with components* $|f_i|$, $\frac{f_i^2}{g_i}$, $|a_{i,j}|$, $\frac{a_{i,j}^2}{p_{i,j}}$, $i, j = 1, \ldots m$, *respectively.*

The following assertions can be found, e.g., in [8, p.289].

**Lemma 2.2** *Let the matrix of the system (2.6) be such that*

$$\varrho(|A|) < 1, \tag{2.12}$$

*where* $\varrho$ *denotes the spectral radius. Assume that the parameters of the Markov chain satisfy (2.9), (2.10) and (2.11). Then the* "**estimator by absorption**", *defined as (cf. (2.8))*

$$\zeta_{abs}(h, A, f)(\omega) = \frac{h_{i_0}\, a_{i_0,i_1} \ldots a_{i_{k-1},i_k}\, f_{i_k}}{\pi_{i_0}\, p_{i_0,i_1} \ldots p_{i_{k-1},i_k}\, g_{i_k}}, \tag{2.13}$$

*is unbiased, i.e.*

$$E\,\zeta_{abs}(h,A,f) = (h,x)\,. \tag{2.14}$$

*Moreover, if*

$$\varrho\left(\frac{A^2}{P}\right) < 1\,, \tag{2.15}$$

*then*

$$E\,[\zeta_{abs}(h,A,f)]^2 = (\frac{h^2}{\pi},\psi)\,, \tag{2.16}$$

*where*

$$\psi = \frac{A^2}{P}\psi + \frac{f^2}{g}\,. \tag{2.17}$$

*Finally,*

$$E\,[\zeta_{abs}(h,A,f)]^2 \geq (|h|,\bar{\varphi})\,. \tag{2.18}$$

*where*

$$\bar{\varphi} = |A|\,\bar{\varphi} + |f|\,. \tag{2.19}$$

**Remark 2.3** *The "***estimator by collisions***" is defined as*

$$\zeta_{coll}(h,A,f)(\omega) = \sum_{l=0}^{k} \frac{h_{i_0}\, a_{i_0,i_1} \cdots a_{i_{l-1},i_l}\, f_{i_l}}{\pi_{i_0}\, p_{i_0,i_1} \cdots p_{i_{l-1},i_l}}\,. \tag{2.20}$$

*If (2.12), (2.9) and (2.10) hold, then*

$$E\,\zeta_{coll}(h,A,f) = (h,x)\,. \tag{2.21}$$

**Remark 2.4** *Note*

$$(h,x) = (f,y)\,, \qquad \textit{where} \qquad y = A^T y + h\,.$$

*Corresponding "adjoint estimators" are obtained by exchanging $h$ and $f$ and replacing $A$ by $A^T$.*

Using unbiased estimators as defined in (2.13) or (2.20), we construct a **random matrix** $\Xi = \Xi(A)$ with elements

$$\xi_{i,j} = \xi_{i,j}(A) = \zeta(e^{(i)}, A, e^{(j)})\,, \qquad i,j = 1,\ldots,m\,,$$

where

$$e_k^{(i)} = \begin{cases} 1\,, & \text{if} \quad k = i\,, \\ 0\,, & \text{otherwise}\,. \end{cases}$$

This matrix satisfies (cf. (2.14), (2.21), (2.7))

$$E\,\Xi(A) = (I - A)^{-1}\,. \tag{2.22}$$

There are different ways to construct $\Xi$.

**Construction 1:** All estimators $\xi_{i,j}$ are defined on one trajectory of the Markov chain (cf. (2.8)). Using the **estimator by absorption** (2.13), we obtain

$$\xi_{i,j}(\omega) = \zeta_{abs}(e^{(i)}, A, e^{(j)})(\omega) = \frac{\delta_{i,i_0}\, a_{i_0,i_1} \ldots a_{i_{k-1},i_k}\, \delta_{j,i_k}}{\pi_{i_0}\, p_{i_0,i_1} \cdots p_{i_{k-1},i_k}\, g_{i_k}}\,, \tag{2.23}$$

where $\delta_{i,j}$ denotes the Kronecker symbol. Here we need condition (2.10) and conditions (cf. (2.9), (2.11))

$$\pi_{min} := \min_i \pi_i > 0\,, \tag{2.24}$$

$$g_{min} := \min_i g_i > 0\,. \tag{2.25}$$

Note that

$$(h, \Xi(A)\, f) = \zeta_{abs}(h, A, f)\,.$$

Since $\xi_{i,j}(\omega) = 0$ if $i_0 \neq i$ or $i_k \neq j$, one obtains

$$\xi_{i,j}(\omega)\, \xi_{\alpha,\beta}(\omega) = 0\,, \qquad \text{if} \quad i \neq \alpha \quad \text{or} \quad j \neq \beta\,. \tag{2.26}$$

Otherwise, one obtains (cf. Remark 2.1)

$$E\,\xi^2_{i,j} = \sum_{k=0}^{\infty} \sum_{i_0,i_1,\ldots,i_k=1}^{m} \frac{\delta_{i,i_0}\, a^2_{i_0,i_1} \ldots a^2_{i_{k-1},i_k}\, \delta_{j,i_k}}{\pi_{i_0}\, p_{i_0,i_1} \cdots p_{i_{k-1},i_k}\, g_{i_k}} = \left(\frac{e^{(i)}}{\pi}, \left(I - \frac{A^2}{P}\right)^{-1} \frac{e^{(j)}}{g}\right). \tag{2.27}$$

**Remark 2.5** *Using the estimator by collisions (2.20) we obtain*

$$\xi_{i,j}(\omega) = \zeta_{coll}(e^{(i)}, A, e^{(j)})(\omega) = \sum_{l=0}^{k} \frac{\delta_{i,i_0}\, a_{i_0,i_1} \ldots a_{i_{l-1},i_l}\, \delta_{j,i_l}}{\pi_{i_0}\, p_{i_0,i_1} \cdots p_{i_{l-1},i_l}} \tag{2.28}$$

*and need the conditions (2.10) and (2.24). Obviously one obtains*

$$\xi_{i,j}(\omega)\, \xi_{\alpha,\beta}(\omega) = 0\,, \qquad \textit{if} \quad i \neq \alpha\,.$$

**Construction 2:** The estimators $\xi_{i,j}$ are defined on a set of $m$ trajectories of the Markov chain, which start at the points $i = 1, \ldots, m$ and are independent. Accordingly we consider

$$\bar{\omega} = \left(\omega^{(1)}, \ldots, \omega^{(m)}\right),$$

where

$$\omega^{(i)} = \left(i, i_1^{(i)}, \ldots, i_{k^{(i)}}^{(i)}\right), \qquad i = 1, \ldots, m\,,$$

and define

$$\xi_{i,j}(\bar{\omega}) = \zeta(e^{(i)}, A, e^{(j)})(\omega^{(i)}) .$$

Independence of the trajectories implies

$$E\,\xi_{i,j}\,\xi_{\alpha,\beta} = E\,\xi_{i,j}\,E\,\xi_{\alpha,\beta} , \qquad i \neq \alpha . \tag{2.29}$$

Using the **estimator by absorption** (2.13), we define (cf. (2.23))

$$\xi_{i,j}(\bar{\omega}) = \zeta_{abs}(e^{(i)}, A, e^{(j)})(\omega^{(i)}) = \frac{a_{i,i_1} \dots a_{i_{k-1},i_k}\,\delta_{j,i_k}}{p_{i,i_1} \dots p_{i_{k-1},i_k}\,g_{i_k}}$$

assuming (2.10) and (2.25). Here we omit the superscript $(i)$. Since $\xi_{i,j}(\bar{\omega}) = 0$, if $i^{(i)}_{k^{(i)}} \neq j$, one obtains

$$\xi_{i,j}\,\xi_{i,l} = 0 , \qquad \text{if} \quad j \neq l . \tag{2.30}$$

Otherwise, one obtains (cf. Remark 2.1)

$$E\,\xi^2_{i,j} = \sum_{k=0}^{\infty} \sum_{i_1,\dots,i_k=1}^{m} \frac{a^2_{i,i_1} \dots a^2_{i_{k-1},i_k}\,\delta_{j,i_k}}{p_{i,i_1} \dots p_{i_{k-1},i_k}\,g_{i_k}} = \left( e^{(i)}, \left( I - \frac{A^2}{P} \right)^{-1} \frac{e^{(j)}}{g} \right) . \tag{2.31}$$

**Remark 2.6** *Using the estimator by collisions (2.20) we define (cf. (2.28))*

$$\xi_{i,j}(\bar{\omega}) = \zeta_{coll}(e^{(i)}, A, e^{(j)})(\omega^{(i)}) = \sum_{l=0}^{k} \frac{a_{i,i_1} \dots a_{i_{l-1},i_l}\,\delta_{j,i_l}}{p_{i,i_1} \dots p_{i_{l-1},i_l}}$$

*and need only condition (2.10).*

## 2.2. Direct Monte Carlo algorithm

Introduce a matrix

$$\mathcal{A}^{(n)} = \begin{pmatrix} A_0 & A_1 & A_2 & \dots & 0 & 0 & 0 \\ 0 & A_0 & A_1 & \dots & 0 & 0 & 0 \\ 0 & 0 & A_0 & \dots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \dots & A_0 & A_1 & A_2 \\ 0 & 0 & 0 & \dots & 0 & A_0 & A_1 \\ 0 & 0 & 0 & \dots & 0 & 0 & A_0 \end{pmatrix}$$

and vectors

$$F^{(n)} = \begin{pmatrix} f \\ f \\ \cdot \\ \cdot \\ f \\ A_2 x^1 + f \\ A_1 x^1 + A_2 x^0 + f \end{pmatrix} , \qquad X^{(n)} = \begin{pmatrix} x^n \\ x^{n-1} \\ \cdot \\ \cdot \\ \cdot \\ x^3 \\ x^2 \end{pmatrix} , \qquad H^{(n,i)} = \begin{pmatrix} e^{(i)} \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}$$

of dimension $m(n-1)$, where $i = 1, \ldots, m$. Then the iteration process (2.1) takes the form (2.6) of a linear algebraic system

$$X^{(n)} = \mathcal{A}^{(n)} X^{(n)} + F^{(n)}, \qquad n \geq 1. \tag{2.32}$$

Applying the von Neumann–Ulam scheme to equation (2.32) one obtains estimates

$$\eta_i^n = \zeta(H^{(n,i)}, \mathcal{A}^{(n)}, F^{(n)}), \qquad i = 1, \ldots, m, \tag{2.33}$$

for the components of $x^n$. We are interested in the behaviour of $\mathrm{Cov}(\eta^n)$ as $n \to \infty$.

We consider the **estimator by absorption** (cf. (2.13)) and a Markov chain with a transition matrix

$$\mathcal{P}^{(n)} = \begin{pmatrix} P_0 & P_1 & P_2 & \ldots & 0 & 0 & 0 \\ 0 & P_0 & P_1 & \ldots & 0 & 0 & 0 \\ 0 & 0 & P_0 & \ldots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \ldots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \ldots & P_0 & P_1 & P_2 \\ 0 & 0 & 0 & \ldots & 0 & P_0 & P_1 \\ 0 & 0 & 0 & \ldots & 0 & 0 & P_0 \end{pmatrix} \tag{2.34}$$

such that conditions analogous to (2.10) and (2.11) are satisfied. Note that conditions (2.12) and (2.15) reduce to (cf. Remark 2.1)

$$\varrho(|A_0|) < 1$$

and

$$\varrho\left(\frac{A_0^2}{P_0}\right) < 1, \tag{2.35}$$

respectively. Condition (2.35) provides finite variance of the estimators (2.33) for fixed $n$.

According to (2.16), (2.17) the second moments of the estimators $\eta_i^n$ are determined by the vector

$$\Psi^{(n)} = \begin{pmatrix} \psi^n \\ \psi^{n-1} \\ \cdot \\ \cdot \\ \cdot \\ \psi^3 \\ \psi^2 \end{pmatrix}$$

satisfying

$$\Psi^{(n)} = \frac{(\mathcal{A}^{(n)})^2}{\mathcal{P}^{(n)}} \Psi^{(n)} + \frac{(F^{(n)})^2}{G^{(n)}}, \tag{2.36}$$

where $G^{(n)}$ is the vector of absorption probabilities corresponding to the transition matrix (2.34). Note that equation (2.36) takes the form

$$\psi^n = \frac{A_0^2}{P_0} \psi^n + \frac{A_1^2}{P_1} \psi^{n-1} + \frac{A_2^2}{P_2} \psi^{n-2} + \frac{f^2}{g}, \qquad n \geq 4,$$

where the vector $g$ is determined by the matrices $P_0, P_1, P_2$. Thus (cf. (2.1), (2.2), (2.4)), a sufficient condition for **stability of the direct procedure** in the sense of (2.5) is

$$\varrho \begin{pmatrix} (I - \frac{A_0^2}{P_0})^{-1} (\frac{A_1^2}{P_1}) & (I - \frac{A_0^2}{P_0})^{-1} (\frac{A_2^2}{P_2}) \\ I & 0 \end{pmatrix} < 1. \tag{2.37}$$

If the choice

$$P_0 = |A_0|, \qquad P_1 = |A_1|, \qquad P_2 = |A_2|$$

is possible then (2.37) reduces to

$$\varrho \begin{pmatrix} (I - |A_0|)^{-1} |A_1| & (I - |A_0|)^{-1} |A_2| \\ I & 0 \end{pmatrix} < 1.$$

From (2.18), (2.19) one obtains the estimate

$$E(\eta_i^n)^2 \geq \bar{\varphi}_i^n, \qquad i = 1, \ldots, m,$$

where

$$\bar{\varphi}^n = |A_0| \, \bar{\varphi}^n + |A_1| \, \bar{\varphi}^{n-1} + |A_2| \, \bar{\varphi}^{n-2} + |f|, \qquad n \geq 4.$$

This provides a sufficient condition for unbounded (exponential) growth of the covariance matrices (at least, for appropriate $f, x^1, x^0$), namely

$$\varrho \begin{pmatrix} (I - |A_0|)^{-1} |A_1| & (I - |A_0|)^{-1} |A_2| \\ I & 0 \end{pmatrix} > 1. \tag{2.38}$$

## 2.3. Recurrent Monte Carlo algorithm

We consider a one-step iteration process

$$x^n = A_0 \, x^n + A_1 \, x^{n-1} + f, \qquad n \geq 1, \tag{2.39}$$

where $x^0 \in \mathcal{R}^m$ is a given initial value. Let $\Xi^n(A_0)$ be a sequence of random matrices such that (cf. (2.22))

$$E_{n-1} \, \Xi^n(A_0) := E \left( \Xi^n(A_0) \mid \mathcal{F}^{n-1} \right) = (I - A_0)^{-1}, \tag{2.40}$$

where $\mathcal{F}^{n-1}$ is the $\sigma$-algebra generated by $\Xi^{n-1}, \ldots, \Xi^1$. Assume that

$$E_{n-1} \, \Delta_{i,j}^n(A_0) \, \Delta_{k,l}^n(A_0) = r_{i,j;k,l}, \tag{2.41}$$

where

$$\Delta^n(A_0) := \Xi^n(A_0) - (I - A_0)^{-1},$$

i.e. that the **covariance matrix** $R(A_0)$ with elements (2.41) is independent of $n$.

We construct a sequence of estimators

$$\eta^0 = x^0, \qquad \eta^n = \Xi^n(A_0) \left[ A_1 \, \eta^{n-1} + f \right], \quad n \geq 1. \tag{2.42}$$

**Lemma 2.7** *If (2.40) holds, then the estimators $\eta^n$ are unbiased, i.e.*

$$E\,\eta^n = x^n\,, \qquad n \geq 0\,. \tag{2.43}$$

**Proof.** Using induction we note that for $n = 0$ the assertion is obviously fulfilled. For $n \geq 1$, one obtains

$$E\,\eta^n = E\,E_{n-1}\,\eta^n = E\,(I - A_0)^{-1}[A_1\,\eta^{n-1} + f] = (I - A_0)^{-1}[A_1\,x^{n-1} + f] = x^n\,,$$

where we used (2.40) and (2.39). ∎

To prepare the formulation of the main result concerning stability of the Monte Carlo procedure, we introduce the following special operations on vectors and matrices. For any vector $y$ of dimension $m$, we define the $m \times m$-matrix $M(y)$ as

$$M(y)_{i,j} := y_i\,y_j\,, \qquad i,j = 1,\ldots,m\,. \tag{2.44}$$

For any $m \times m$-matrix $B$, we denote by $\overrightarrow{B}$ the corresponding vector of length $m^2$, i.e.

$$(\overrightarrow{B})_{i,j} := b_{i,j}\,, \qquad i,j = 1,\ldots,m\,, \tag{2.45}$$

and by $\mathcal{M}(B)$ the $m^2 \times m^2$-matrix defined as

$$\mathcal{M}(B)_{i,j;k,l} = b_{i,k}\,b_{j,l}\,, \qquad i,j,k,l = 1,\ldots,m\,. \tag{2.46}$$

The following theorem provides an explicit formula for the sequence of covariance matrices.

**Theorem 2.8** *Assume (2.40) and (2.41). Then, for all $n \geq 1$,*

$$\overrightarrow{\mathrm{Cov}(\eta^n)} = \sum_{k=0}^{n-1} \Big[\mathcal{M}((I - A_0)^{-1}\,A_1) + \tilde{R}(A_0)\,\mathcal{M}(A_1)\Big]^k\,\tilde{R}(A_0)\,\overrightarrow{M((I - A_0)\,x^{n-k})}\,, \tag{2.47}$$

*where $\tilde{R}(A_0)$ is a matrix with elements*

$$\tilde{r}_{i,j;\alpha,\beta} := r_{i,\alpha;j,\beta}\,, \qquad i,j,\alpha,\beta = 1,\ldots,m\,. \tag{2.48}$$

The family of random matrices $\Xi^n(A_0)$, which determines the sequence of estimators $\eta^n$, is characterized by the covariance matrix $R(A_0)$. According to Theorem 2.8, the sequence of estimators $\eta^n$ is stable in the sense of (2.5) if and only if the covariance matrix $R(A_0)$ and the sequence $x^n$ are such that the right-hand side of (2.47) is bounded.

The behaviour of the random error $\eta^n - x^n$ for large $n$ depends on the spectral properties of the operator $S = \mathcal{M}((I - A_0)^{-1}\,A_1) + \tilde{R}(A_0)\,\mathcal{M}(A_1)$. If the sequence $x^n$ is bounded, then stability follows from the condition $\varrho(S) < 1$. In the case $\varrho(S) > 1$, the random errors accumulate and the norm of the covariance matrices grows, in general, exponentially fast. These conclusions equally apply to finite iteration processes of the form (2.39), which occur if a solution to a partial differential equation is calculated on a finite time interval using some difference scheme (see the examples in the next section).

It turns out that a stable Monte Carlo procedure can be constructed based on any family of random matrices $\Xi^n(A_0)$ satisfying (2.40) and (2.41).

**Corollary 2.9** *Let the estimators $\Xi^n(A_0)$ be averaged over $N$ independent samples. Assume that the sequence $x^n$ is bounded. If*

$$\varrho((I - A_0)^{-1} A_1) < 1 \tag{2.49}$$

*and $N$ is sufficiently large, then the recurrent algorithm (2.42) is stable in the sense of (2.5).*

**Remark 2.10** *For the two-step iteration process (2.1) condition (2.49) takes the form (cf. (2.3), (2.4))*

$$\varrho\left((\mathcal{I} - \mathcal{A}_0)^{-1} \mathcal{A}_1\right) < 1 .$$

*Thus, the stability condition for the recurrent procedure is identical to the standard convergence condition for the iteration process (2.1).*

The proofs of the above assertions are prepared by several lemmas.

**Lemma 2.11** *For any matrix $B$,*

$$\varrho(\mathcal{M}(B)) = \varrho(B)^2 . \tag{2.50}$$

**Proof.** For any $m \times m$-matrices $B, C$ one obtains

$$[B\,C\,B^T]_{i,j} = \sum_{k=1}^{m} b_{i,k}\,[C\,B^T]_{k,j} = \sum_{k,l=1}^{m} b_{i,k}\,b_{j,l}\,c_{k,l}$$

and therefore according to (2.45), (2.46)

$$\overrightarrow{B\,C\,B^T} = \mathcal{M}(B)\,\overrightarrow{C} . \tag{2.51}$$

From

$$\begin{aligned}[\mathcal{M}(B)\,\mathcal{M}(C)]_{i,j;k,l} &= \sum_{\alpha,\beta} \mathcal{M}(B)_{i,j;\alpha,\beta}\,\mathcal{M}(C)_{\alpha,\beta;k,l} = \sum_{\alpha,\beta} b_{i,\alpha}\,b_{j,\beta}\,c_{\alpha,k}\,c_{\beta,l} \\ &= (B\,C)_{i,k}\,(B\,C)_{j,l} = \mathcal{M}(B\,C)_{i,j;k,l}\end{aligned}$$

one obtains

$$\mathcal{M}(B)\,\mathcal{M}(C) = \mathcal{M}(B\,C) .$$

For any vectors $y, z$ of dimension $m$, we define the $m \times m$-matrix $M_1(y,z)$ as

$$M_1(y,z)_{i,j} := y_i\,z_j , \qquad i,j = 1,\dots,m . \tag{2.52}$$

Assume

$$B\,y = \lambda\,y , \qquad B\,z = \mu\,z .$$

Then according to (2.51), (2.52)

$$\left[\mathcal{M}(B)\,\overrightarrow{M_1(y,z)}\right]_{i,j} = [B\,M_1(y,z)\,B^T]_{i,j} = \sum_{k,l} b_{i,k}\,y_k\,z_l\,b_{j,l} = \lambda\,\mu\,y_i\,z_j , \qquad i,j = 1,\dots,m ,$$

so that

$$\mathcal{M}(B)\,\overrightarrow{M_1(y,z)} = \lambda\,\mu\,\overrightarrow{M_1(y,z)}$$

and (2.50) follows. ∎

**Lemma 2.12** *If* $\varrho(B) < 1$ *then there exists* $\delta > 0$ *such that* $\|\Delta B\| < \delta$ *implies* $\varrho(B + \Delta B) < 1$.

**Proof.** This property is known as "upper semicontinuity" of the spectral radius (cf., e.g., [20, Cor. 2.4.3]). ■

**Lemma 2.13** *Consider a sequence* $y^n = B\,y^{n-1} + \psi^n$, $n \geq 1$, $y^0 \in \mathcal{R}^m$. *If* $\varrho(B) < 1$ *and* $\sup_n \|\psi^n\| < \infty$, *then* $\sup_n \|y^n\| < \infty$.

**Proof.** The result follows from the representation $y^n = B^j\,y^{n-j} + \sum_{i=0}^{j-1} B^i\,\psi^{n-i}$, and the fact that $\|B^j\| < 1$, for some $j$ and an appropriate norm. ■

**Proof of Theorem 2.8.** Consider the stochastic error

$$\varepsilon^n := \eta^n - x^n\,, \qquad n \geq 1\,, \tag{2.53}$$

which satisfies

$$\begin{aligned} \varepsilon^n &= \Xi^n(A_0)\,A_1\,\varepsilon^{n-1} + \Xi^n(A_0)\,[A_1\,x^{n-1} + f] - x^n \\ &= (I - A_0)^{-1}\,A_1\,\varepsilon^{n-1} + \Delta^n(A_0)\,A_1\,\varepsilon^{n-1} + \Delta^n(A_0)\,[A_1\,x^{n-1} + f]\,. \end{aligned} \tag{2.54}$$

Note that (cf. (2.41))

$$E\sum_{j=1}^m \Delta_{i,j}^n\,a_j \sum_{l=1}^m \Delta_{k,l}^n\,b_l = E\sum_{j,l=1}^m a_j\,b_l\,E_{n-1}\,\Delta_{i,j}^n\,\Delta_{k,l}^n = \sum_{j,l=1}^m r_{i,j;k,l}\,E\,a_j\,b_l\,, \tag{2.55}$$

if the vectors $a, b$ are $\mathcal{F}^{n-1}$-measurable. The first term in (2.54) and the rest of the sum are uncorrelated, since $E_{n-1}\,\Delta^n(A_0) = 0$. The second and the third term are uncorrelated according to (2.55), since $E\,A_1\varepsilon^{n-1} = 0$. Thus, (2.54) implies

$$\begin{aligned} &\mathrm{Cov}(\varepsilon^n) = \\ &\quad \mathrm{Cov}((I - A_0)^{-1}\,A_1\,\varepsilon^{n-1}) + \mathrm{Cov}(\Delta^n(A_0)\,A_1\,\varepsilon^{n-1}) + \mathrm{Cov}(\Delta^n(A_0)\,[A_1\,x^{n-1} + f])\,. \end{aligned} \tag{2.56}$$

Note that

$$\mathrm{Cov}(B\,\varepsilon^{n-1}) = B\,\mathrm{Cov}(\varepsilon^{n-1})\,B^T\,. \tag{2.57}$$

Using (2.55) one obtains

$$\mathrm{Cov}_{i,k}(\Delta^n(A_0)\,A_1\,\varepsilon^{n-1}) = \sum_{j,l=1}^m r_{i,j;k,l}\,\mathrm{Cov}_{j,l}(A_1\,\varepsilon^{n-1}) \tag{2.58}$$

and (cf. (2.1))

$$\mathrm{Cov}_{i,k}(\Delta^n(A_0)\,[A_1\,x^{n-1} + f]) = \sum_{j,l=1}^m r_{i,j;k,l}\,[(I - A_0)\,x^n]_j\,[(I - A_0)\,x^n]_l\,. \tag{2.59}$$

According to (2.45), (2.44) and (2.48), the identities (2.58), (2.59) imply

$$\overrightarrow{\mathrm{Cov}(\Delta^n(A_0)\,A_1\,\varepsilon^{n-1})} = \tilde{R}(A_0)\,\overrightarrow{\mathrm{Cov}(A_1\,\varepsilon^{n-1})} \tag{2.60}$$

and

$$\overrightarrow{\mathrm{Cov}(\Delta^n(A_0)\,[A_1\,x^{n-1}+f])} = \tilde{R}(A_0)\,\overrightarrow{M((I-A_0)\,x^n)}\,. \tag{2.61}$$

Note that $\mathrm{Cov}(\eta^n) = \mathrm{Cov}(\varepsilon^n)$, according to (2.43) and (2.53). Using (2.57), (2.60), (2.61) and (2.51), equation (2.56) takes the form

$$\overrightarrow{\mathrm{Cov}(\eta^n)} = \left[\mathcal{M}((I-A_0)^{-1}\,A_1) + \tilde{R}(A_0)\,\mathcal{M}(A_1)\right]\overrightarrow{\mathrm{Cov}(\eta^{n-1})} + \tilde{R}(A_0)\,\overrightarrow{M((I-A_0)\,x^n)}\,,$$

and (2.47) follows. Note that $\mathrm{Cov}(\eta^0) = 0$ according to (2.42). ■

**Proof of Corollary 2.9.** If the estimators $\Xi^n(A_0)$ are averaged over $N$ independent samples, then $\tilde{R}(A_0)$ is replaced by $\frac{1}{N}\,\tilde{R}(A_0)$. Using (2.49) and (2.50), we apply Lemma 2.12 with $B = \mathcal{M}((I-A_0)^{-1}\,A_1)$ and $\Delta B = \frac{1}{N}\,\tilde{R}(A_0)\,\mathcal{M}(A_1)$. Thus, the result follows from Lemma 2.13 with $B = \mathcal{M}((I-A_0)^{-1}\,A_1) + \tilde{R}(A_0)\,\mathcal{M}(A_1)$ and $\psi^n = \tilde{R}(A_0)\,\overrightarrow{M((I-A_0)\,x^n)}$, and the boundedness of $x^n$. ■

Finishing this section we consider some special cases and analyze the matrix $\tilde{R}(A_0)$ that appears in (2.47). Considering the norm $\|B\| = \max_i \sum_j |b_{i,j}|$, and using the definitions (2.48), (2.41), one obtains

$$\|\tilde{R}(A_0)\| = \max_{i,j} \sum_{k,l} \left|E_{n-1}\,\xi^n_{i,k}\,\xi^n_{j,l} - E_{n-1}\xi^n_{i,k}\,E_{n-1}\xi^n_{j,l}\right|. \tag{2.62}$$

where $\xi^n_{i,j}$ denote the components of the matrices $\Xi^n$. In case of **construction 1** and the estimator by absorption (2.23), one obtains from (2.26), (2.40) and (2.27)

$$\begin{aligned}\|\tilde{R}(A_0)\| &\le \max_i \sum_k E_{n-1}\,[\xi^n_{i,k}]^2 + \|\mathcal{M}((I-A_0)^{-1})\| \\ &\le \pi^{-1}_{min}\,g^{-1}_{min}\left\|\left(I-\frac{A_0^2}{P_0}\right)^{-1}\right\| + \|\mathcal{M}((I-A_0)^{-1})\|\,.\end{aligned} \tag{2.63}$$

In case of **construction 2** one obtains from (2.62), (2.29)

$$\begin{aligned}\|\tilde{R}(A_0)\| &\le \max_i \sum_{k,l} \left|E_{n-1}\,\xi^n_{i,k}\,\xi^n_{i,l}\right| + \max_{i\neq j} \sum_{k,l} \left|E_{n-1}\,\xi^n_{i,k}\,E_{n-1}\,\xi^n_{i,l}\right| \\ &\le \max_i \sum_{k,l} \left|E_{n-1}\,\xi^n_{i,k}\,\xi^n_{i,l}\right| + \|\mathcal{M}((I-A_0)^{-1})\|\,.\end{aligned}$$

For the estimator by absorption one obtains from (2.30) and (2.31)

$$\|\tilde{R}(A_0)\| \le g^{-1}_{min}\left\|\left(I-\frac{A_0^2}{P_0}\right)^{-1}\right\| + \|\mathcal{M}((I-A_0)^{-1})\|\,. \tag{2.64}$$

From the definition (2.46) one obtains

$$\|\mathcal{M}(B)\| = \max_{i,j} \sum_{k,l} |\mathcal{M}(B)_{i,j;k,l}| = \max_{i,j} \sum_{k,l} |b_{i,k}|\,|b_{j,l}| \le \|B\|^2\,. \tag{2.65}$$

Assuming

$$\|A_0\| < 1 \quad \text{and} \quad P_0 = A_0\,,$$

one obtains $\|(I - A_0)^{-1}\| \le \frac{1}{1-\|A_0\|}$ and $g_{min} \ge 1 - \|A_0\|$, so that

$$\|\tilde{R}(A_0)\| \le \frac{c}{(1 - \|A_0\|)^2}, \tag{2.66}$$

where $c = \pi_{min}^{-1} + 1$ in case of construction 1 (cf. (2.63)) and $c = 2$ in case of construction 2 (cf. (2.64)).

Finally, it follows from (2.66), (2.65) that

$$N > \frac{c\,\|A_1\|^2}{\delta\,(1 - \|A_0\|)^2} \tag{2.67}$$

is sufficient to assure $\|\frac{1}{N}\,\tilde{R}(A_0)\,\mathcal{M}(A_1)\| < \delta$ (cf. Lemma 2.12). However, the estimate (2.67) is too rough to be useful in practical calculations, since in general $\delta$ may be very small. In the symmetric case one may obtain a more explicit estimate for $N$, using $\delta = 1 - \varrho((I - A_0)^{-1} A_1)^2$ (cf. (2.49)) and some appropriate norm.

# 3. Application to difference schemes

## 3.1. Wave equation

Consider the one-dimensional wave equation

$$\frac{\partial^2}{\partial t^2} u(t,x) = \frac{\partial^2}{\partial x^2} u(t,x),$$

where $x \in [0,1]$ and $t \ge 0$, with the initial conditions

$$u(0,x) = u_0(x), \quad (\frac{\partial}{\partial t} u)(0,x) = u_1(x) \tag{3.1}$$

and the boundary conditions

$$u(t,0) = 0, \quad u(t,1) = 0. \tag{3.2}$$

Let

$$h = \frac{1}{m+1} \tag{3.3}$$

be the discretization parameter in the space $[0,1]$, and $\tau$ the discrete time step. Difference schemes are defined using a grid function

$$\hat{u}(j\tau, kh), \qquad j = 0,1,\ldots,n, \qquad k = 0,1,\ldots m+1.$$

We denote

$$y_k^j := \hat{u}(j\tau, kh), \qquad j = 0,1,\ldots,n, \qquad k = 0,1,\ldots m+1,$$

and define, using the initial and boundary conditions (3.1), (3.2),

$$y_k^0 = u_0(k\,h), \qquad k = 0,\ldots,m+1,$$

$$y_k^1 = u_0(k\,h) + \tau\, u_1(k\,h)\,, \qquad k = 0, \ldots, m+1\,,$$

and

$$y_0^j = 0\,, \qquad y_{m+1}^j = 0\,, \qquad j = 0, 1, \ldots, n\,.$$

It remains to determine the vectors

$$y^j = (y_1^j, \ldots, y_m^j)\,, \qquad j = 2, \ldots, n\,.$$

We introduce the second order **difference operator**

$$(\Delta_h\, z)_k := \frac{z_{k+1} - 2\,z_k + z_{k-1}}{h^2}\,, \qquad k = 1, \ldots, m\,, \tag{3.4}$$

acting on vectors $z = (z_1, \ldots, z_m)$, where $z_0 = z_{m+1} := 0$. This operator takes the form

$$\Delta_h\, z = \frac{1}{h^2}\,(B - 2\,I)\,z\,, \tag{3.5}$$

where

$$B = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 & 0 \\ 1 & 0 & 1 & \ldots & 0 & 0 \\ 0 & 1 & 0 & \ldots & 0 & 0 \\ \cdot & \cdot & \cdot & \ldots & \cdot & \cdot \\ 0 & 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & 0 & \ldots & 1 & 0 \end{pmatrix}.$$

This matrix has eigenvalues (cf., e.g., [17, p. 67])

$$2 + \lambda_l\,, \quad \text{where} \quad \lambda_l = -4\,\sin^2\left(\frac{\pi\,l}{2\,(m+1)}\right)\,, \qquad l = 1, \ldots, m\,, \tag{3.6}$$

and eigenvectors

$$v_k^{(l)} := \sin\frac{\pi\,k\,l}{m+1}\,, \qquad k, l = 1, \ldots, m\,.$$

Note that (cf. (3.3))

$$-4 < -4\,\sin^2\frac{\pi}{2}\,(1-h) \;\le\; \lambda_l \;\le\; -4\,\sin^2\frac{\pi}{2}\,h < 0\,, \qquad l = 1, \ldots, m\,. \tag{3.7}$$

Consider a three-layer **difference scheme** of the form

$$\frac{y_k^{j+1} - 2\,y_k^j + y_k^{j-1}}{\tau^2} = \alpha\,(\Delta_h\, y^{j+1})_k + \beta\,(\Delta_h\, y^j)_k + \gamma\,(\Delta_h\, y^{j-1})_k\,, \tag{3.8}$$

where $j \ge 1\,, \quad k = 1, \ldots, m\,,$ and $\alpha, \beta, \gamma$ are non-negative weights such that

$$\alpha + \beta + \gamma = 1\,. \tag{3.9}$$

From (3.8) and (3.5) one obtains

$$\frac{h^2}{\tau^2}\left(y^{j+1} - 2\,y^j + y^{j-1}\right) = \alpha\,(B - 2\,I)\,y^{j+1} + \beta\,(B - 2\,I)\,y^j + \gamma\,(B - 2\,I)\,y^{j-1},$$

$$(2\,\alpha + \frac{h^2}{\tau^2})\,y^{j+1} = B\,y^{j+1} + \left[2\,\frac{h^2}{\tau^2}\,I + \beta\,(B - 2\,I)\right] y^j + \left[\gamma\,(B - 2\,I) - \frac{h^2}{\tau^2}\,I\right] y^{j-1},$$

and finally

$$y^{j+1} = A_0\,y^{j+1} + A_1\,y^j + A_2\,y^{j-1},$$

where

$$A_0 = \frac{\alpha}{2\,\alpha + \mu^2}\,B, \tag{3.10}$$

$$A_1 = \frac{2\,[\mu^2 - \beta]}{2\,\alpha + \mu^2}\,I + \frac{\beta}{2\,\alpha + \mu^2}\,B, \tag{3.11}$$

$$A_2 = -\frac{\mu^2 + 2\,\gamma}{2\,\alpha + \mu^2}\,I + \frac{\gamma}{2\,\alpha + \mu^2}\,B, \tag{3.12}$$

and

$$\mu^2 := \frac{h^2}{\tau^2}. \tag{3.13}$$

Thus, the vectors $y^j$ are determined by an iteration process of the form (2.1).

According to Remark 2.10, the condition for **stability of the recurrent procedure** is

$$\varrho(\mathcal{B}) < 1,$$

where (cf. (2.4))

$$\mathcal{B} = \begin{pmatrix} (I - A_0)^{-1}\,A_1 & (I - A_0)^{-1}\,A_2 \\ I & 0 \end{pmatrix}. \tag{3.14}$$

Note that $|A_0| = A_0$, $|A_1| = A_1$, if $\mu^2 \geq \beta$, and $|A_2| \neq A_2$.

**Lemma 3.1** *Consider $A_0$ from (3.10) and*

$$A_1 = \frac{\varepsilon_1}{2\,\alpha + \mu^2}\,I + \frac{\beta}{2\,\alpha + \mu^2}\,B, \tag{3.15}$$

$$A_2 = \frac{\varepsilon_2}{2\,\alpha + \mu^2}\,I + \frac{\gamma}{2\,\alpha + \mu^2}\,B. \tag{3.16}$$

*For $\mathcal{B}$ defined in (3.14), one obtains*

$$\varrho(\mathcal{B}) = \max_l |\eta_l^{(1,2)}|, \tag{3.17}$$

*where*

$$\eta_l^{(1,2)} = \frac{\varepsilon_1 + (2 + \lambda_l)\,\beta \pm \sqrt{[\varepsilon_1 + (2 + \lambda_l)\,\beta]^2 + 4\,[\mu^2 - \lambda_l\,\alpha]\,[\varepsilon_2 + (2 + \lambda_l)\,\gamma]}}{2\,[\mu^2 - \lambda_l\,\alpha]}. \tag{3.18}$$

**Corollary 3.2** *In the case* $\varepsilon_1 = 2[\mu^2 - \beta]$, $\varepsilon_2 = -(\mu^2 + 2\gamma)$ *one obtains*

$$\eta_l^{(1,2)} = \frac{2\mu^2 + \lambda_l \beta \pm \sqrt{\lambda_l^2(\beta^2 - 4\gamma\alpha) + 4\lambda_l \mu^2}}{2[\mu^2 - \lambda_l \alpha]}. \tag{3.19}$$

**Corollary 3.3** *In the special case*

$$\beta = 0, \quad \gamma = 1 - \alpha, \tag{3.20}$$

*one obtains*

$$\left|\eta_l^{(1,2)}\right| = \sqrt{1 - \frac{\lambda_l(1-2\alpha)}{\mu^2 - \lambda_l \alpha}} \tag{3.21}$$

*so that*

$$\begin{aligned} &\varrho(\mathcal{B}) < 1 \quad \text{if} \quad \alpha > \tfrac{1}{2}, \\ &\varrho(\mathcal{B}) = 1 \quad \text{if} \quad \alpha = \tfrac{1}{2}, \\ &\varrho(\mathcal{B}) > 1 \quad \text{if} \quad \alpha < \tfrac{1}{2}. \end{aligned}$$

Proofs are given in the Appendix.

**Example 3.4 (Standard implicit scheme "T")** *In the* **special case**

$$\alpha = 1, \quad \beta = 0, \quad \gamma = 0,$$

*one obtains from (3.21)*

$$\left|\eta_l^{(1,2)}\right| = \frac{\mu}{\sqrt{\mu^2 - \lambda_l}}$$

*and (cf. (3.7), [22, p.263])*

$$\varrho(\mathcal{B}) = \frac{\mu}{\sqrt{\mu^2 + 4\sin^2(\frac{\pi h}{2})}} < 1.$$

*Using* $\sin^2 x \sim x^2$, $\frac{1}{\sqrt{1+x^2}} \sim 1 - \frac{x^2}{2}$ $(x \to 0)$, *and taking into account (3.13), one obtains*

$$\varrho(\mathcal{B}) \sim 1 - \frac{\pi^2}{2\mu^2} h^2 = 1 - \frac{\pi^2}{2} \tau^2.$$

*This implies stability of the* **recurrent procedure**.

*Note that (cf. (3.10)-(3.12))*

$$A_0 = \frac{1}{2+\mu^2} B, \qquad A_1 = \frac{2\mu^2}{2+\mu^2} I, \qquad A_2 = -\frac{\mu^2}{2+\mu^2} I.$$

*One obtains (cf. (2.2))*

$$\|\mathcal{A}_0\| = \frac{2}{2+\mu^2}, \qquad \|\mathcal{A}_1\| = \begin{cases} 1, & \text{if} \quad \mu < 1, \\ \frac{3\mu^2}{2+\mu^2}, & \text{if} \quad \mu \geq 1, \end{cases}$$

*and (cf. (2.67))*

$$\frac{\|\mathcal{A}_1\|}{1-\|\mathcal{A}_0\|} = \begin{cases} 1+\frac{2}{\mu^2}, & \text{if } \mu<1, \\ 3, & \text{if } \mu \geq 1. \end{cases}$$

*However, the variance of the* **direct procedure** *is unbounded with respect to* $n$. *Note that* $|A_2|$ *corresponds to* $\varepsilon_2 = \mu^2$ *and (3.18) implies (with* $\varepsilon_1 = 2\mu^2$*)*

$$\eta_l^{(1,2)} = \frac{2\mu^2 \pm \sqrt{4\mu^4 + 4[\mu^2-\lambda_l]\mu^2}}{2[\mu^2-\lambda_l]} = \frac{\mu^2 \pm \mu\sqrt{2\mu^2-\lambda_l}}{\mu^2-\lambda_l}.$$

*Since the function* $\frac{1+\sqrt{2+x}}{1+x}$ *is decreasing, one obtains*

$$\max_l \left|\eta_l^{(1,2)}\right| = \frac{\mu^2+\mu\sqrt{2\mu^2+4\sin^2(\frac{\pi h}{2})}}{\mu^2+4\sin^2(\frac{\pi h}{2})} \sim 1+\sqrt{2},$$

*and (2.38) is fulfilled.*

**Example 3.5 (Standard explicit scheme "Cross")** *In the* **special case**

$$\beta = 1, \quad \alpha = 0, \quad \gamma = 0,$$

*one obtains from (3.19)*

$$\eta_l^{(1,2)} = \frac{2\mu^2+\lambda_l \pm \sqrt{\lambda_l^2+4\lambda_l\mu^2}}{2\mu^2} = 1+\frac{\lambda_l}{2\mu^2} \pm \sqrt{\left(1+\frac{\lambda_l}{2\mu^2}\right)^2-1}.$$

*If* $\left|1+\frac{\lambda_l}{2\mu^2}\right| > 1$, *for some* $l$, *then* $\varrho(\mathcal{B}) > 1$. *If*

$$\left|1+\frac{\lambda_l}{2\mu^2}\right| \leq 1, \qquad \forall l, \tag{3.22}$$

*then*

$$\varrho(\mathcal{B}) = 1.$$

*According to (3.6) we have* $\lambda_l \in (-4,0)$ *so that a sufficient condition for (3.22) is* $1-\frac{4}{2\mu^2} \geq -1$ *or* $\mu^2 \geq 1$, *i.e. (cf. (3.13)) ([22, p.263])*

$$\tau \leq h.$$

*Note that (cf. (3.10)-(3.12))*

$$A_0 = 0, \qquad A_1 = \frac{2[\mu^2-1]}{\mu^2} I + \frac{1}{\mu^2} B, \qquad A_2 = -I.$$

*The* **recurrent procedure** *degenerates to a deterministic algorithm, since the choice* $\mathcal{P}_0 = \mathcal{A}_0$ *corresponds to immediate absorption with probability 1.*

*The* **direct procedure** *has a variance unbounded with respect to* $n$. *Note that* $|A_1| = A_1$ *(if* $\mu^2 \geq 1$*) and* $|A_2|$ *corresponds to* $\varepsilon_2 = \mu^2$ *and (3.18) implies (with* $\varepsilon_1 = 2(\mu^2-1)$*)*

$$\eta_l^{(1,2)} = \frac{2\mu^2+\lambda_l \pm \sqrt{(2\mu^2+\lambda_l)^2+4\mu^4}}{2\mu^2}$$

*and*

$$\max_l \left|\eta_l^{(1,2)}\right| \sim 1+\sqrt{2}$$

*so that (2.38) holds.*

## 3.2. Heat flow equation

Consider the one-dimensional heat flow equation

$$\frac{\partial}{\partial t} u(t,x) = \frac{\partial^2}{\partial x^2} u(t,x)\,,$$

where $x \in [0,1]$ and $t \geq 0$, with the initial condition

$$u(0,x) = u_0(x)$$

and the boundary conditions

$$u(t,0) = 0\,, \quad u(t,1) = 0\,.$$

Let $h = \frac{1}{m+1}$ be the discretization parameter in the space $[0,1]$, and $\tau$ the discrete time step. Define

$$y_k^0 = u_0(k\,h)\,, \quad k = 0,\ldots,m+1\,,$$

and

$$y_0^j = 0\,, \quad y_{m+1}^j = 0\,, \quad j \geq 0\,.$$

Consider a **difference scheme** with weights (cf., e.g., [22, p.17] or [25, p.321])

$$\frac{y_k^{j+1} - y_k^j}{\tau} = \sigma\,(\Delta_h\, y^{j+1})_k + (1-\sigma)\,(\Delta_h\, y^j)_k\,, \qquad j \geq 0\,, \quad k = 1,\ldots,m\,, \tag{3.23}$$

where $\sigma \in [0,1]$ and $\Delta_h$ is defined in (3.4). From (3.23) and (3.5) one obtains

$$\frac{h^2}{\tau}\,(y^{j+1} - y^j) = \sigma\,(B - 2\,I)\,y^{j+1} + (1-\sigma)\,(B - 2\,I)\,y^j$$

and

$$y^{j+1} = A_0\,y^{j+1} + A_1\,y^j\,,$$

where

$$A_0 = \frac{\sigma}{2\,\sigma + \mu^2}\,B\,, \qquad A_1 = \frac{(1-\sigma)}{2\,\sigma + \mu^2}\,B + \frac{\mu^2 - 2\,(1-\sigma)}{2\,\sigma + \mu^2}\,I\,, \tag{3.24}$$

and

$$\mu^2 := \frac{h^2}{\tau}\,. \tag{3.25}$$

Thus, the vectors $y^j$ are determined by an iteration process of the form (2.1).

The condition for **stability of the recurrent procedure** is (cf. (2.49))

$$\varrho((I - A_0)^{-1}\,A_1) < 1\,. \tag{3.26}$$

**Lemma 3.6** *One obtains*

$$\varrho((I - A_0)^{-1} A_1) = \max_l |\eta_l| , \tag{3.27}$$

*where*

$$\eta_l = \frac{(1-\sigma)\,\lambda_l + \mu^2}{-\sigma\,\lambda_l + \mu^2} . \tag{3.28}$$

The proof is given in the Appendix.

According to (3.6) we have $\lambda_l \in (-4, 0)$ so that $\eta_l < 1$. On the other hand one obtains from (3.28)

$$\begin{aligned} \eta_l > -1 \quad &\Longleftrightarrow \quad (1-\sigma)\,\lambda_l + \mu^2 > \sigma\,\lambda_l - \mu^2 \\ &\Longleftrightarrow \quad (1-2\sigma)\,\lambda_l + 2\,\mu^2 > 0 , \end{aligned}$$

which is fulfilled (cf. (3.7), [22, p.18]) if $\sigma \in [\frac{1}{2}, 1]$ or if

$$\mu^2 = \frac{h^2}{\tau} \geq 2\,(1 - 2\,\sigma) \quad \text{and} \quad \sigma \in [0, \frac{1}{2}) . \tag{3.29}$$

Thus, condition (3.26) holds for $\sigma \in [\frac{1}{2}, 1]$ or if (3.29) is fulfilled.

**Example 3.7 (Implicit scheme)** *In the case $\sigma = 1$ formula (3.28) takes the form*

$$\eta_l = \frac{\mu^2}{-\lambda_l + \mu^2}$$

*so that, according to (3.7),*

$$\varrho((I - A_0)^{-1} A_1) = \frac{\mu^2}{4\,\sin^2(\frac{\pi}{2}\,h) + \mu^2} < 1 .$$

*Using* $\sin^2 x \sim x^2$, $\frac{1}{1+x} \sim 1 - x$ $(x \to 0)$, *and taking into account (3.25), one obtains*

$$\varrho((I - A_0)^{-1} A_1) \;\sim\; 1 - \frac{\pi^2}{\mu^2}\,h^2 = 1 - \pi^2\,\tau .$$

*Note that (cf. (3.24))*

$$A_0 = \frac{1}{2 + \mu^2}\,B , \qquad A_1 = \frac{\mu^2}{2 + \mu^2}\,I$$

*and there is no sign change. Thus, the stability conditions for the* **direct** *and the* **recurrent algorithm** *are identical. One obtains (cf. (2.67))*

$$\|A_0\| = \frac{2}{2 + \mu^2} , \qquad \|A_1\| = \frac{\mu^2}{2 + \mu^2} , \qquad \frac{\|A_1\|}{1 - \|A_0\|} = 1 .$$

**Example 3.8 (Explicit scheme)** *In the case $\sigma = 0$ condition (3.29) takes the form*

$$\mu^2 = \frac{h^2}{\tau} \geq 2\,. \tag{3.30}$$

*Formula (3.28) takes the form*

$$\eta_l = \frac{\mu^2 + \lambda_l}{\mu^2}$$

*so that, according to (3.27) and (3.7),*

$$\varrho((I - A_0)^{-1}A_1) = 1 - \frac{4}{\mu^2}\sin^2(\frac{\pi}{2}h) < 1$$

*and*

$$\varrho((I - A_0)^{-1}A_1) \;\sim\; 1 - \pi^2\tau\,.$$

*Note that (cf. (3.24))*

$$A_0 = 0\,, \qquad A_1 = \frac{1}{\mu^2}B + \frac{\mu^2 - 2}{\mu^2}I$$

*and there is no sign change in the case (3.30). The* **recurrent procedure** *degenerates to a deterministic algorithm. The stability condition for the* **direct procedure** *is fulfilled.*

## 3.3. Numerical examples

Here we study the simplest implicit scheme for the wave equation (cf. Example 3.4) in order to illustrate the theoretical results concerning stability of the recurrent procedure. On each time step, averaging over $N$ independent samples is used (cf. Corollary 2.9).

First we calculate the solution up to time $t = 1.$ in order to illustrate the qualitative behaviour of the Monte Carlo procedure. The results are obtained by a single run of the algorithm. The parameters of the difference scheme are $h = \tau = 0.02$. The figures below show three typical situations. In Figure 1 ($N = 100$) we observe stability and negligible stochastic errors. In Figure 2 ($N = 10$) the procedure is still stable, but the stochastic fluctuations start to play some role. Finally, in Figure 3 ($N = 4$) the stochastic error becomes predominant, and the procedure is unstable.

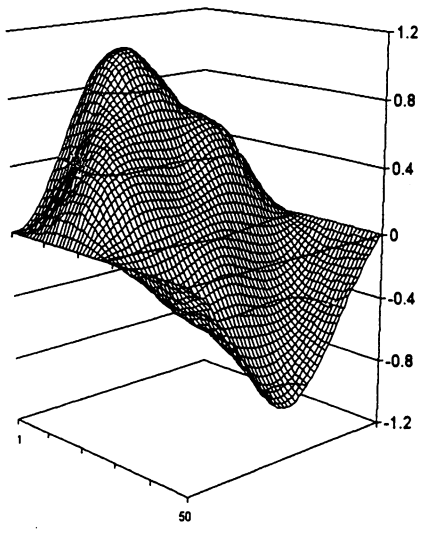


**Figure 1** Stability with small random error ($N = 100$)

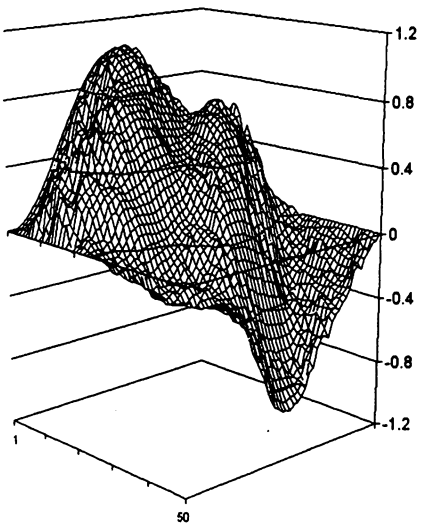


**Figure 2** Stability with moderate random error ($N = 10$)

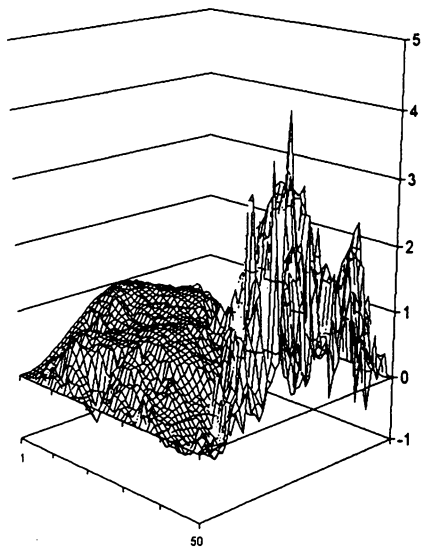


**Figure 3** Instability ($N = 4$)

Next we present some results illustrating the quantitative behaviour of the random error. The numbers shown in the tables are determined by the formula

$$\sqrt{\frac{1}{m}\sum_{i=1}^{m}\mathrm{Var}(\eta_i^n)}\,. \tag{3.1}$$

The variances of the component estimators are approximated using averaging over independent runs of the procedure.

First we consider the case $h = \tau = 0.02$. The values (3.1) for different $N$ on small time intervals are shown in Table 1.

**Table 1**

| N | $t = 1.$ | $t = 2.$ |
|---|---|---|
| 100 | 0.032 | 0.035 |
| 50 | 0.050 | 0.057 |
| 25 | 0.075 | 0.093 |
| 20 | 0.089 | 0.110 |
| 10 | 0.173 | 0.232 |
| 8 | 0.242 | 0.345 |
| 5 | 0.775 | 2.44 |
| 4 | 2.70 | 29.2 |
| 2 | 2.51E+4 | 1.15E+10 |
| 1 | 2.85E+10 | 5.46E+22 |

These results allow us to conclude that instability occurs for $N = 1$ and $N = 2$. To make a more precise conclusion, we calculate the values (3.1) on longer time intervals. The results from Table 2 show that the procedure is stable for $N = 8$.

**Table 2**

| N | $t = 4.$ | $t = 10.$ | $t = 100.$ |
|---|---|---|---|
| 8 | 0.823 | 0.888 | 0.757 |
| 7 | 0.611 | 3.29 | 100245. |
| 6 | 1.12 | 15.9 | 4.74E+11 |

Next we consider the case $h = \tau = 0.01$. The corresponding results are given in Tables 3 and 4. In this case the procedure becomes stable only for $N = 12$.

**Table 3**

| N | $t = 1.$ | $t = 2.$ |
|---|---|---|
| 100 | 0.031 | 0.049 |
| 50 | 0.053 | 0.061 |
| 25 | 0.086 | 0.121 |
| 10 | 0.218 | 0.386 |
| 5 | 2.25 | 20.0 |

**Table 4**

| N | $t = 4.$ | $t = 10.$ | $t = 100.$ | t=1000. |
|---|---|---|---|---|
| 12 | 0.323 | 0.468 | 4.56 | 2.78. |
| 11 | 0.437 | 2.05 | 16.7 | 4.59E+11 |
| 10 | 0.739 | 4.46 | 16766. | |
| 9 | 1.09 | 1.39 | 21378. | |
| 8 | 0.808 | 4.39 | 2.04E+12 | |

Finally, the result for the case $h = \tau = 0.005$ are shown in Tables 5 and 6. Here the procedure is stable for from $N = 18$.

**Table 5**

| N | L | $t = 1.$ | $t = 2.$ |
|---|---|---|---|
| 50 | 20 | 0.053 | 0.077 |
| 25 | 40 | 0.092 | 0.122 |
| 20 | 50 | 0.130 | 0.175 |
| 10 | 100 | 0.296 | 0.690 |
| 5 | 200 | 15.8 | 1552. |

**Table 6**

| N | $t = 4.$ | $t = 10.$ | $t = 100.$ | $t = 1000.$ |
|---|---|---|---|---|
| 19 | 0.267 | 0.486 | 4.19 | 0.036 |
| 18 | 0.183 | 0.377 | 7.66 | 0.035 |
| 17 | 0.325 | 0.376 | 68.4 | 9.94E+10 |
| 15 | 0.351 | 0.994 | 167. | 1.49E+17 |
| 12 | 0.774 | 4.15 | 3.05E+06 | |

The number $N$, for which the Monte Carlo procedure is stable, increases with a decreasing time step. This behaviour is in accordance with the theoretical predictions. However, the actual numbers observed in the numerical tests are much less than the upper estimates obtained in Section 2 (cf. (2.67) and Example 3.4).

# 4. Conclusions

The main concern of this paper was the study of stability properties of Monte Carlo algorithms for iteration processes. As a basic illustration, the problem of constructing stable Monte Carlo procedures for the wave equation has been considered. A solution to this problem is provided by the recurrent Monte Carlo algorithm studied in Section 2.3.

As it follows from the main theorem, there exists some $N$, the number of trajectories on each time layer, which is sufficient to make the algorithm stable in the sense of uniformly bounded variances. One of the important features of Monte Carlo algorithms is their highly efficient implementation on parallel computer architectures. This is due to the fact that independent samples of the corresponding random estimator can be generated on different processors. As we observed in Section 3.1, the direct Monte Carlo algorithm with independent trajectories (cf. Section 2.2) does not work successfully in the case of difference schemes for the wave equation. The variances of the estimators grow exponentially fast, leading to poor efficiency. For the recurrent Monte Carlo algorithm, instead of using $M = L\,N$ independent trajectories in the direct scheme, $N$ of them are used in a form splitted over the time layers. The whole procedure is then repeated $L$ times independently and the final result is obtained by averaging. The $L$ independent runs can be again distributed very efficiently among different processors. Moreover, if $L$ is sufficiently large to apply the central limit theorem, confidence intervals for the solution of the problem can be constructed. As the numerical examples show, the number $N$ need not to be very large in applied problems.

Numerical experiments have been carried out for the one-dimensional wave equation. This allowed us to investigate the effects of stability and instability more explicitly. The theoretical results of Section 2, however, apply to the wave equation in more than one dimension (cf. [13], [26]). Thus, the range of applicability of the Monte Carlo method has been extended by the recurrent algorithms proposed in this paper. It is subject of future work to find more precise estimates of the necessary number of averaging steps $N$ in the multi-dimensional case (cf. the remarks at the end of Section 2). This would allow us to compare the new Monte Carlo algorithm and conventional deterministic methods with respect to their computational efficiency.

It would be of interest to check the procedure for difference schemes for the wave equation with discontinuous coefficients (cf. [3]). Monte Carlo algorithms are especially well-suited in situations, where equations with random coefficients are to be solved numerically (cf. [24]), so that wave propagation in random media (cf. [21]) is an interesting field of application. The principal ideas concerning stability can be applied to more general iteration processes, when the matrices $A_0, A_1, A_2$ and vectors $f$ in (2.1) depend on the iteration step. Further improvements of the approach in the spirit of Halton's sequential Monte Carlo (cf. [15]) seem to be possible.

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# Appendix

**Proof of Lemma 3.1.** If one assumes

$$\begin{pmatrix} (I-A_0)^{-1}A_1 & (I-A_0)^{-1}A_2 \\ I & 0 \end{pmatrix} \begin{pmatrix} z \\ w \end{pmatrix} = \eta \begin{pmatrix} z \\ w \end{pmatrix}$$

then

$$(I-A_0)^{-1}A_1 z + (I-A_0)^{-1}A_2 w = \eta z\,, \qquad z = \eta w\,,$$

which implies

$$(I-A_0)^{-1}A_1 \eta w + (I-A_0)^{-1}A_2 w = \eta^2 w\,.$$

and

$$A_1 \eta w + A_2 w = \eta^2 (I-A_0) w\,. \tag{A.1}$$

Taking into account (3.10), (3.15), (3.16) one obtains from (A.1)

$$\eta^2 \left[I - \frac{\alpha}{2\alpha+\mu^2} B\right] w = \eta \left[\frac{\varepsilon_1}{2\alpha+\mu^2} I + \frac{\beta}{2\alpha+\mu^2} B\right] w + \left[\frac{\varepsilon_2}{2\alpha+\mu^2} I + \frac{\gamma}{2\alpha+\mu^2} B\right] w$$

and

$$\left[\eta^2 \frac{\alpha}{2\alpha+\mu^2} + \eta \frac{\beta}{2\alpha+\mu^2} + \frac{\gamma}{2\alpha+\mu^2}\right] B w = \left[\eta^2 - \eta \frac{\varepsilon_1}{2\alpha+\mu^2} - \frac{\varepsilon_2}{2\alpha+\mu^2}\right] w\,.$$

According to (3.6) $\eta$ must satisfy

$$\left[\eta^2 \frac{\alpha}{2\alpha+\mu^2} + \eta \frac{\beta}{2\alpha+\mu^2} + \frac{\gamma}{2\alpha+\mu^2}\right] (2+\lambda_l) = \eta^2 - \eta \frac{\varepsilon_1}{2\alpha+\mu^2} - \frac{\varepsilon_2}{2\alpha+\mu^2}\,,$$

$$\eta^2 \frac{\lambda_l \alpha - \mu^2}{2\alpha+\mu^2} + \eta \frac{\varepsilon_1 + (2+\lambda_l)\beta}{2\alpha+\mu^2} + \frac{\varepsilon_2 + (2+\lambda_l)\gamma}{2\alpha+\mu^2} = 0$$

or

$$\eta^2 + \eta \frac{\varepsilon_1 + (2+\lambda_l)\beta}{\lambda_l \alpha - \mu^2} + \frac{\varepsilon_2 + (2+\lambda_l)\gamma}{\lambda_l \alpha - \mu^2} = 0$$

Note that $\lambda_l < 0$ (cf. (3.7)). Thus, (3.17) follows. ■

**Proof of Corollary 3.2.** Using (3.9) one obtains

$$[2\mu^2 + \beta\lambda_l]^2 + 4[\mu^2 - \lambda_l \alpha][-\mu^2 + \lambda_l \gamma] = 4\mu^2 \beta \lambda_l + \beta^2 \lambda_l^2 + 4\mu^2 \lambda_l \gamma + 4\mu^2 \lambda_l \alpha - 4\lambda_l^2 \alpha\gamma = 4\mu^2 \lambda_l + \lambda_l^2 (\beta^2 - 4\alpha\gamma)$$

and (3.19) follows. ■

**Proof of Corollary 3.3.** In the case (3.20) one obtains from (3.19)

$$\eta_l^{(1,2)} = \frac{2\mu^2 \pm \sqrt{-4\lambda_l^2(1-\alpha)\alpha + 4\lambda_l\mu^2}}{2[\mu^2 - \lambda_l\alpha]} = \frac{\mu^2 \pm \sqrt{-\lambda_l^2(1-\alpha)\alpha + \lambda_l\mu^2}}{\mu^2 - \lambda_l\alpha}.$$

According to (3.6) this implies

$$\begin{aligned}\left|\eta_l^{(1,2)}\right| &= \frac{\sqrt{\mu^4 + \lambda_l^2(1-\alpha)\alpha - \lambda_l\mu^2}}{\mu^2 - \lambda_l\alpha} \\ &= \frac{\sqrt{(\mu^2 - \lambda_l\alpha)^2 + \lambda_l(2\alpha-1)\mu^2 + \lambda_l^2(1-2\alpha)\alpha}}{\mu^2 - \lambda_l\alpha} \\ &= \frac{\sqrt{(\mu^2 - \lambda_l\alpha)^2 + (1-2\alpha)\lambda_l[\lambda_l\alpha - \mu^2]}}{\mu^2 - \lambda_l\alpha} \\ &= \sqrt{\frac{\mu^2 - \lambda_l\alpha - (1-2\alpha)\lambda_l}{\mu^2 - \lambda_l\alpha}} = \sqrt{1 - \frac{(1-2\alpha)\lambda_l}{\mu^2 - \lambda_l\alpha}}\end{aligned}$$

so that (3.21) follows. ■

**Proof of Lemma 3.6.** If one assumes

$$(I - A_0)^{-1} A_1 w = \eta w,$$

then

$$A_1 w = \eta w - A_0 \eta w$$

and according to (3.24)

$$\frac{1-\sigma}{2\sigma + \mu^2} B w + \frac{\mu^2 - 2(1-\sigma)}{2\sigma + \mu^2} w = \eta w - \frac{\sigma}{2\sigma + \mu^2} \eta B w$$

or

$$\frac{1 - \sigma + \sigma\eta}{2\sigma + \mu^2} B w = \left(\eta - \frac{\mu^2 - 2(1-\sigma)}{2\sigma + \mu^2}\right) w.$$

According to (3.7) $\eta$ must satisfy (for some $l$)

$$\frac{1 - \sigma + \sigma\eta}{2\sigma + \mu^2}(2 + \lambda_l) = \eta - \frac{\mu^2 - 2(1-\sigma)}{2\sigma + \mu^2},$$

$$\frac{1-\sigma}{2\sigma + \mu^2}(2 + \lambda_l) + \frac{\mu^2 - 2(1-\sigma)}{2\sigma + \mu^2} = \eta\left(1 - \frac{\sigma}{2\sigma + \mu^2}(2 + \lambda_l)\right)$$

or

$$(1-\sigma)\lambda_l + \mu^2 = \eta[2\sigma + \mu^2 - \sigma(2 + \lambda_l)].$$

Thus, one obtains (3.28). ■

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